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Numerical Studies on Flow Behavior of Composite Propellant Slurry During Vacuum Casting

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Abstract: Rockets are powered by composite solid propellant, which is a heterogeneous system consisting of solid oxidizer and metallic fuel dispersed in a polymeric fuel binder matrix. The slurry casting technique under vacuum/gravity condition is well-established for performing a different class of large sized case bonded rocket motors. During propellant casting, the flow rate of slurry is a very critical parameter as it affects the product quality. The casting rate is governed by sufficient degassing and viscosity buildup due to the progress of cure reaction. In the present study, casting rate and casting time have been numerically evaluated for fixed and varying percentages of valve opening, different viscosity of slurry, and different pressure drop (driving force). The velocity profile of propellant slurry inside feeding pipe and valve has also been evaluated. Furthermore, to get a flawless grain and to predict the slurry casting rate, a microscopic analysis has been carried out to model the flow behaviour of composite propellant slurry, where the momentum conservation law has been applied to express the mathematical model in an analytical form. The resulting differential and algebraic equations have been solved numerically using MATLAB, computing software. The numerical analysis is useful for designing new casting set-up and for giving the idea of maximum casting rate, which is achievable for given casting set-up and rheological properties of propellant slurry.

Keywords: Microscopic analysis, Composite propellant, Vacuum casting, Casting rate, Casting time.

LIST OF SYMBOLS

ΔP	Pressure drop	N/m ²
V_{avg}	Average velocity	m/s
a	Percentage opening of the valve	%
h	Slurry height in the bowl	m
V	Volume	m ³
μ	Viscosity	Pa.S
N_{Re}	Reynolds number	

INTRODUCTION

Composite propellants (CP) are the most important class of solid rocket propellant used in various missile programmes and space applications. A CP consists of an inorganic oxidizer such as ammonium perchlorate (65 to 70%), a metallic fuel

such as aluminum powder (15 to 20%), and a polymeric binder such as hydroxyl terminated poly-butadiene (10 to 12%) along with certain isocyanate based curatives and process aids (Boyers and Klager, 1969). The main objective of propellant processing is to produce flawless propellant grain; therefore, special precautions are taken in application of vacuum and control of slurry flow rate (casting rate), during propellant casting. Several techniques are adopted worldwide for the casting of propellants, viz., vacuum casting, pressure casting, bayonet casting, etc (Davenas, 1993; Krishnan and Ghokhale, 1993). Among these, a suitable casting method is chosen based on parameters like type of propellant, rheological behavior of propellant slurry, and web size and grain geometry of rocket motors (Muthiah and Krishnamurthy, 1996).

Vacuum/gravity casting is the most widely adopted technique for propellant casting. Propellant slurry is introduced inside a rocket motor from the mixer bowl through feed pipe and control valve. The driving force for flow of propellant slurry is gravitational force and vacuum inside casting chamber. The casting rate of slurry is an important parameter in determining product quality, which mainly depends upon

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rheological behavior of slurry, pot life of propellant, and flow path available for casting. Propellant slurry behaves as a pseudo-plastic, thixotropic fluid and its rheological behavior is modeled as the power law fluid model (Mahanta *et al.*, 2010). Few studies on modeling and simulation of propellant casting are reported in literature. The pressure drop determination during pressure casting was carried out by Dombe *et al.* (2008). The 3D unsteady flow field and free surface movement during solid propellant casting were simulated by Rafi *et al.* (2010). Dormaus *et al.* (1988) have developed a computer model for the distribution prediction of solid particle constituents during casting of propellant in rocket motor. Shimada *et al.* (2007) have also used bidirectional X-ray penetration measurement and digital image analysis for estimation of propellant slurry velocity field during vacuum casting.

During propellant processing, propellant formulations with different burning rates (4 to 40 mm/s @ 70 ksc) result in propellant slurry, with different rheological properties (end of mix viscosity, pseudo-plasticity index, etc). Also, the flow path available for casting (web thickness) of propellant grain varies based on the grain geometry. Therefore, processing of wide variety of propellant formulations, with different web thicknesses, is essential to find out the variation in slurry flow rate with percentage opening of valve with different rheological characteristics. Furthermore, to predict casting rate and duration of vacuum casting with % opening of control valve (ball valve), mathematical modeling and simulation of casting set up are carried out where momentum balance equations are applied across various components of casting system and related equations have been solved numerically using a code written in MATLAB. The material used in simulation for propellant consist of ammonium perchlorate (68%), aluminum powder (18%), hydroxyl terminated polybutadiene (13%), toluene diisocyanate (0.7%), and process aids.

In the following section, we have reported the results of numerical studies on velocity distribution, mass flow rate, casting rate, pressure drop, slurry height in mixer bowl during vacuum casting, as well as the influence of viscosity on these parameters.

MATHEMATICAL MODELING

During the mathematical modeling, momentum balance equations are formulated for several components of casting system. The pressure drop for each component is added to get the overall pressure drop. The momentum conservation law

has been applied over a shell of the slurry having infinitesimal dimension followed by the integration over the whole control volume of the casting system, which provides the required momentum equation. Following assumptions have been made for the mathematical modeling:

- steady state one-dimensional laminar flow;
- continuum flow behavior;
- pseudo-plastic behavior obeying power law;
- fully developed flow;
- no-slip boundary condition;
- constant properties of the slurry throughout casting;
- circular free surface of slurry inside the valve.

MOMENTUM BALANCE EQUATION FOR VARIOUS COMPONENTS OF CASTING SYSTEM

The momentum balance equations are derived for the following four components of casting system. The various components of the casting system, as depicted in Fig. 1, are discussed below.

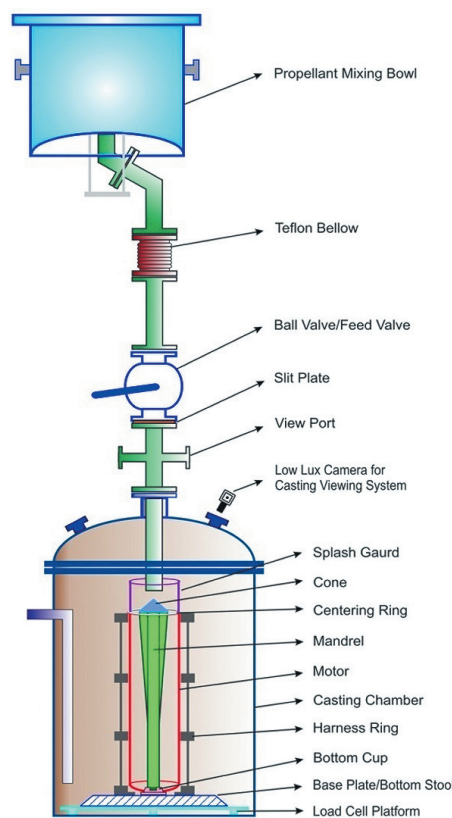


Figure 1. Schematic diagram of casting set-up.

Slanted and straight pipe-I

For flows through pipe with the assumption of fully developed flow, no-slip boundary condition and pseudo-plastic nature of slurry with power law behavior, slurry velocity, volumetric flow rate, and average velocity are expressed as Eqs. 1 to 3 (Mathews and Fink, 2006):

$$V_y = M[1 - (x/R)^{\frac{1}{n+1}}], \text{ where } M = \frac{n}{n+1} \left(\frac{\Delta P}{2KL} \right)^{1/n} R^{\frac{1}{n+1}} \quad (1)$$

$$Q = \int V_y dA, A = \pi x^2 \Rightarrow Q = \frac{n\pi}{3n+1} \left(\frac{\Delta P}{2KL} \right)^{1/n} R^{\frac{3n+1}{n}} \quad (2)$$

$$V_{avg} = \frac{Q}{\pi R^2} = \frac{n}{3n+1} \left(\frac{\Delta P}{2KL} \right)^{1/n} R^{\frac{n+1}{n}} \quad (3)$$

where:

ΔP is overall pressure drop inclusive of gravitation head. For slanted pipe, $\cos\theta$ component of gravitational head is considered.

Fluids obeying power law, Reynolds number is expressed as (Saleh, 2002):

$$N_{Re} = \frac{\rho V_{avg}^{2-n} D^n}{8^{n-1} K \left(\frac{3n+1}{4n} \right)^n} \quad (4)$$

Ball valve

For modeling flow through ball valve, consider a circular shell (Fig. 2) having thickness Δx at a distance of x from the centre of sphere (ball valve). Momentum balance equation across the thickness Δx is expressed as (Bird *et al.*, 2002):

$$[\{\tau_{xy} \pi z^2\}_x - \{\tau_{xy} \pi z^2\}_{x+\Delta x}] + [(P_3 - P_4) 2\pi z \Delta x + \pi z^2 \Delta x \rho g \cos \theta] = 0 \quad (5)$$

$$\frac{d}{dx} [z^2 \tau_{xy}] = 2z \Delta P_3 + z^2 x \rho g \cos \theta$$

If z is the radius of circular shell and r is the distance of shell from the centre of sphere:

$$x^2 + z^2 = R^2 \quad (6)$$

Then;

$$(R^2 - x^2) \tau_{xy} = 2\Delta P_3 [R^2 \sin^{-1}(x/R) + x\sqrt{R^2 - x^2}] + \rho g \cos \theta [R^2 x - x^3/3] + C_1 \quad (7)$$

With no-slip boundary condition, τ_{xy} = finite at $x = R$, it becomes:

$$C_1 = -2\Delta P_3 R^2 \frac{\pi}{2} + \rho g \cos \theta 2R^3/3 \quad (8)$$

$$\frac{dV_y}{dx} = \left[\frac{\{2\Delta P_3 [R^2 \sin^{-1}(x/R) + x\sqrt{R^2 - x^2}] + \rho g \cos \theta [R^2 x - x^3/3] + C_1\}}{K(R^2 - x^2)} \right]^{1/n} \quad (9)$$

For obtaining r -value, a circular shell of fluid in the ball valve is considered (Fig. 3), in which volume in the first octant is given as

$$\begin{aligned} vol &= \iiint z \, dx \, dy, \text{ where } x^2 + y^2 + z^2 = R^2 \\ &= \int_r^R \int_0^{\sqrt{R^2 - x^2}} \sqrt{R^2 - x^2 - y^2} \, dy \, dx = \frac{\pi}{4} \int_r^R (R^2 - x^2) \, dx \\ &= \pi/4 \left[\frac{2R^3}{3} - R^2 r \right] + \frac{r^3}{3} = \frac{\pi}{4} \int_r^R (R^2 - x^2) \, dx \\ &= \pi/4 \left[\frac{2R^3}{3} - R^2 r \right] + \frac{r^3}{3} \end{aligned} \quad (10)$$

Volume of slurry in the valve is $V = 4 \times vol$. If percentage opening of the valve is α , this volume will be $\alpha/100$ of

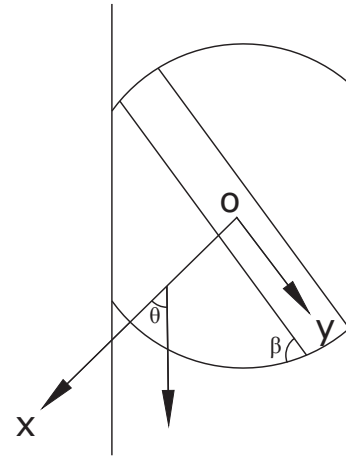


Figure 2. Schematic diagram of the ball valve.

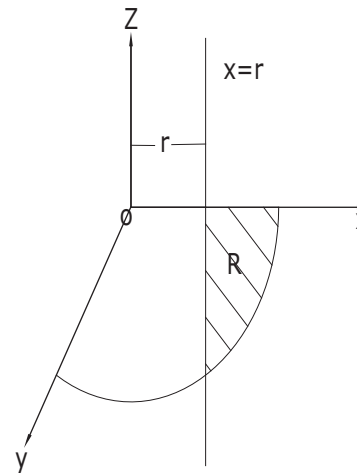


Figure 3. Circular shell of fluid in ball valve.

the total volume:

$$\frac{\pi}{3}[r^3 - 3R^2r + 2R^3] = \frac{\alpha}{100} \times \frac{4}{3} \pi R^3 \quad (11)$$

$$r^3 - 3R^2r + (2 - \alpha/25)R^3 = 0, \text{ where } 0 < r < R$$

Straight pipe II

The straight pipe II is a partially filled pipe (Fig. 4). For modeling flow through this pipe, consider a shell of slurry at a distance x from the centre of pipe having thickness Δx . If r is the distance of shell from the centre of pipe, momentum balance equation can be expressed (Bird *et al.*, 2002) as:

$$[\{\tau_{xy} 2zL_3\}_x - \{\tau_{xy} 2zL_3\}_{x+\Delta x}] + 2z\Delta xL_3\rho g + (P_4 - P_3) 2z\Delta x = 0$$

$$z\tau_{xy} = \frac{\Delta P_4}{2} [R^2 \sin^{-1}(x/R) + x\sqrt{R^2 - x^2}] + C_1 \quad (12)$$

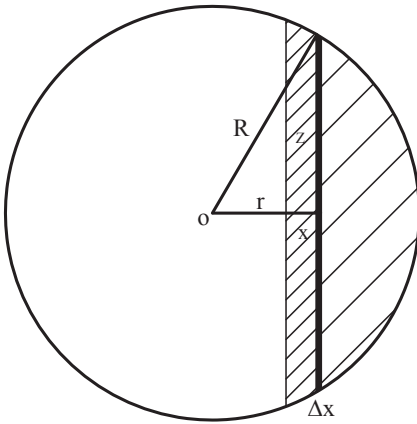


Figure 4. Section of straight pipe after ball valve.

With no-slip boundary condition, i.e., $\tau_{xy} = \text{finite at } x = R$:

$$\frac{dV_y}{dx} = \left(\frac{\Delta P_4}{2K} \right)^{1/n} \left[\frac{[R^2 \sin^{-1}(x/R) + x\sqrt{R^2 - x^2}] - R^2 \frac{\pi}{2}}{\sqrt{R^2 - x^2}} \right]^{1/n} \quad (13)$$

For obtaining the r -value, a circular shell of fluid in straight pipe II is considered (Fig. 5). If percentage of the pipe flow area will be occupied by slurry, an area of the shaded part will be:

$$\frac{1}{2} \times \frac{\alpha}{100} \pi R^2$$

$$\int_r^R y dx = \int_r^R \sqrt{R^2 - x^2} dx = \frac{1}{2} \times \frac{\alpha}{100} \pi R^2$$

$$\theta + \frac{1}{2} \sin 2\theta = \frac{100 - 2\alpha}{200} \pi, 0 < \theta < \frac{\pi}{2} \quad (14)$$

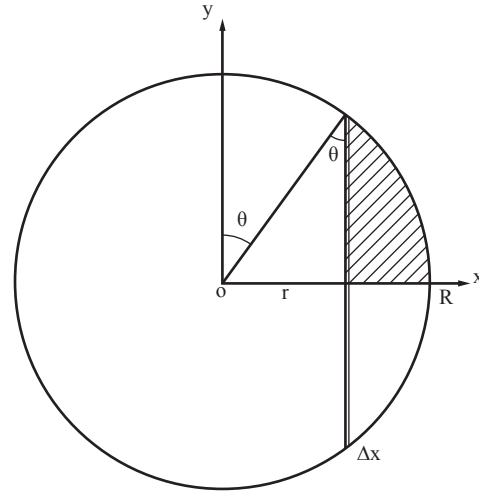


Figure 5. Shell of fluid inside straight pipe II.

Modeling of slurry height in bowl

Slurry height in the bowl is modeled using continuity equation and assuming constant properties of the slurry for the casting setup, by considering one surface as a free one of slurry in the bowl and another one as flow surface of slurry in straight pipe after the ball valve:

$$h = h_0 - \left(\frac{A_4 V_4}{A} \right) t \quad (15)$$

Equation 15 provides a variation of the propellant slurry height in a bowl at any time.

RESULTS AND DISCUSSION

A computational software called MATLAB has been used to carry out numerical simulations of differential and algebraic Eqs. 1 to 15 governing the propellant flow during vacuum casting (Mathews and Fink, 2006). Newton-Raphson method was used to solve the equations for which initial values were obtained from the bisection method (Chapra and Canale, 2005). For the numerical analysis, propellant properties used were: specific gravity of propellant slurry of 1.75 g/cc; initial height of propellant slurry in the bowl of 0.45 m; unit shear viscosity of propellant slurry of 330 Pa.s; pseudo-plasticity index (n) of 0.8 and vacuum level inside the motor of 3 torr. Casting time was evaluated based on time required for 950 kg casting of propellant slurry into the rocket motor.

The various flow parameters, such as casting rate, average and maximum velocity, velocity profiles inside various components, were obtained numerically for a given % opening of ball valve and pressure drop. These parameters were obtained from several % opening of valve varying from 0 to 35%.

Effect of pressure drop on mass flow rate

The results of numerical simulation in terms of overall pressure drop, average and maximum velocity in pipes, and casting time are presented in Table 1. It is clear that the overall pressure drop varies linearly with the mass flow rate for a constant valve opening. The variation of pressure drop with mass flow rate is given in Fig. 6, which indicates linear variation of pressure drop with mass flow rate. It is found that increase in mass flow rate from 10 to 25 kg/hr increases pressure drop from 46,505 to 95,878 Pa.

Table 1. Variation of pressure drop with mass flow rate.

Mass flow rate (kg/min)	Pressure drop (Pa)	Average velocity (m/s)	Max velocity (m/s)	Time (minutes)
10	46505	0.0054	0.0101	95
11	50121	0.0059	0.0111	87
12	53686	0.0064	0.0121	80
13	57155	0.0070	0.0132	73
14	60615	0.0075	0.0142	68
15	63980	0.0080	0.0152	64
18	73884	0.0096	0.0182	53
20	80280	0.0107	0.0202	48
25	95878	0.0134	0.0253	38

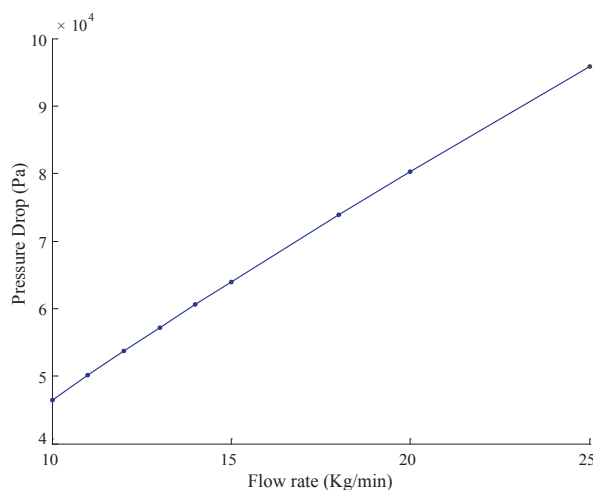


Figure 6. Variation of pressure drop with mass flow rate.

Velocity distribution inside various components of casting system

The velocity distribution inside straight pipes I and II, ball valve are given in Figs. 7 to 9. The velocity distribution in straight pipe I for propellant slurry indicates that the curve is not exactly parabolic which is attributed to the pseudo-plasticity nature ($n=0.8$) of the propellant slurry. The velocity distribution inside ball valve of propellant slurry indicates that the maximum velocity of the propellant slurry is at the free surface of slurry inside the valve, and decreases towards the valve surface, whereas velocity of the slurry is zero at the surface of the valve. The velocity distribution of propellant slurry in the pipe after ball valve also indicates that the maximum velocity is at the free surface of slurry inside the pipe. It is found that increase in mass flow rate from 10 to 25 kg/hr increases average velocity from 5.4×10^{-3} to 13.4×10^{-3} m/s. Reynold's number for the propellant slurry during casting is calculated, which is of the order of 10^{-3} , indicating flow to be creeping flow.

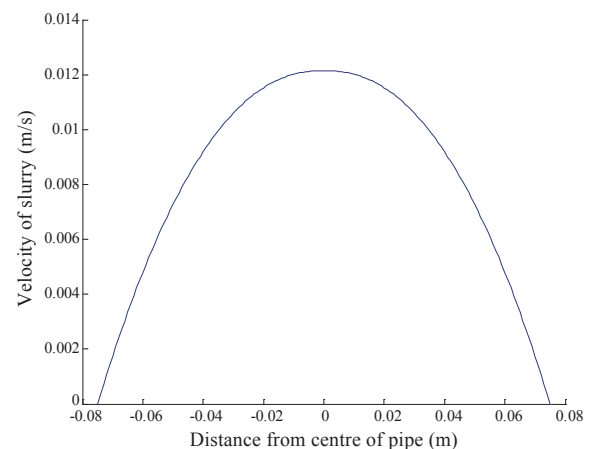


Figure 7. Velocity distribution inside pipe I.

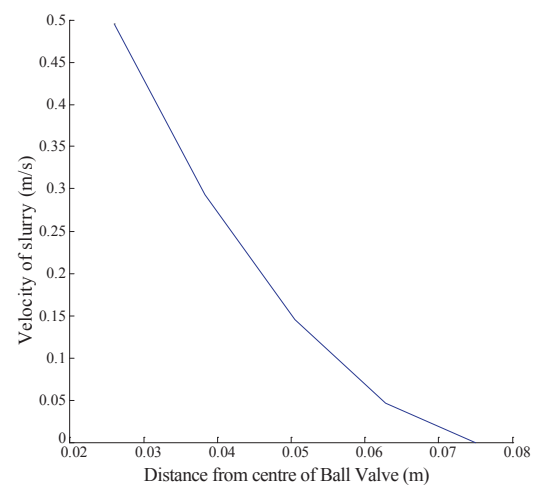


Figure 8. Velocity distribution inside ball valve.

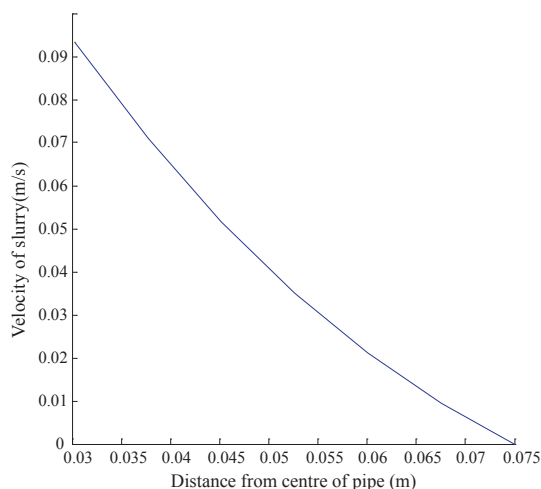


Figure 9. Velocity distribution inside pipe II.

Influence of viscosity on pressure drop and casting time

Influence of viscosity on pressure drop for fixed mass flow rate is given in Fig. 10. It was found that as viscosity increases, the pressure drop linearly increases. The overall pressure drop varies from 28,450 to 82,340 Pa for viscosity values in the range of 500 to 1,500 Pas. Further, it was found that as viscosity increases, casting time increases for constant % valve of opening.

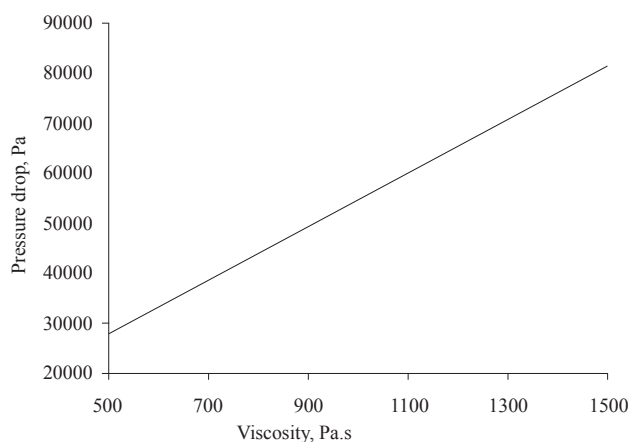


Figure 10. Variation of pressure drop with viscosity.

Influence of percentage opening of valve on pressure drop

Influence of percentage opening of valve on pressure drop is given in Fig. 11. It was found that pressure drop increases with a decrease in percentage opening of valve. The pressure drop observed for 15% opening of valve is 8.5×10^4 Pa. The pressure drop for 35% and above opening of valve is 4.6×10^4 Pa.

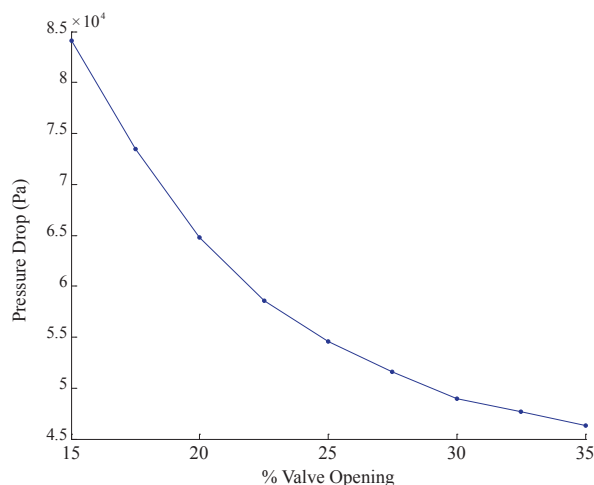


Figure 11. Variation of pressure drop with valve opening.

CONCLUSIONS

The flow behavior of CP slurry during vacuum casting has been numerically modeled in terms of differential and algebraic equations, which are formulated using numerically microscopic analysis. The governing equations are simulated to study the behavior of slurry flow rate on overall pressure drop and the time taken by the slurry to reach inside motor from the bowl for fixed and varying percentages of valve opening. This numerical analysis of casting system is useful in designing new casting setup and gives the idea of maximum casting rate achievable for a certain casting setup and rheological properties of slurry. This relation is very useful for deciding % opening of valve for attaining given casting rate for propellant slurry, with different unit shear viscosity.

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